CENTER FOR COMPUTATIONAL MATERIALS SCIENCE

- The Center conducts theoretical and computational research on the electronic and physical properties of diverse condensed matter systems. These include metals, semiconductors, and insulators, in ordered and disordered states and in alloy configurations. Modern mathematical and numerical techniques are used to study static and dynamic properties of condensed phases and cluster systems, and the interaction of radiation with atoms and matter.

- Major research efforts include: electronic, phononic, magnetic, optical, and mechanical characteristics of matter; transport properties; phase transformations; defect behavior and superconductivity in materials; and the interaction of radiation with atoms and solids. Our techniques include first-principles electronic-structure methods, tight-binding methods, molecular dynamics, numerical statistical-mechanical methods, quantum many-body theory, and density-matrix methods.

- Supercomputers and modern visualization techniques are utilized to facilitate comparison with existing experimental results, and to predict or guide experiments.

- The research has strong couplings with Navy experimental research programs and, in many cases, has the capability for predicting new materials with enhanced properties.

RESEARCH AREAS

Computational Methods The Center supports the Office of Naval Research's Grand Challenge "Navy Materials by Design," by developing and maintaining a variety of computational tools. These include first-principles methods based on density-functional theory, specialized models for highly correlated systems, efficient tight-binding and over-lapping-atom models, and simulation methods spanning multiple length scales.

Disordered Systems We study the nature of vibrons in disordered systems of various types using modeling and supercell methods. The characterization of normal modes in disordered crystals, glasses, amorphous materials, and materials with crystalline amorphous interfaces gives insight into thermal conduction and vibrational spectroscopic properties.

Ferroelectrics Ferroelectric perovskites play a key role in Navy technology, particularly the transducers (sound producing and detecting elements) in SONAR arrays, electronic applications and microwave circuits. We are using computational methods to understand the properties of these materials on an atomic-level basis, and are using this to identify avenues for improving existing materials and to find new superior compositions.

Magnetic Materials The Center studies a broad range of magnetic materials, from bulk materials to molecular magnets to magnetic semiconductors. Some of these materials form the basis of current magnetoelectronic technologies, while others — both soft and hard magnets — are being studied for future applications.

Magnetic Semiconductors This research focuses on dilute magnetic semiconductors, a new class of materials in which magnetic dopants are used to create ferromagnets from normal semiconductors such as GaAs. These materials, which offer the advantages of semiconductors combined with the non-volatile properties of magnetic materials, are the materials foundation for future "spintronics" technologies.

Molecules and Clusters We predict how molecules and clusters respond when subjected to mechanical, electro-magnetic, or chemical probes. Our interest is in exploiting properties which allow for information storage, environmental sensing, or energy conversion. This work is accomplished by predicting stabilities, reactivities, geometries, electronic and vibrational spectra, and magnetic properties.

Mechanical Properties We apply computational methods including first principles, tight binding, and coupling of length scales approaches to the simulation of mechanical properties. Applications range from static calculations of quantities such as ideal strength and ductility criteria, to dynamic simulations of finite-temperature ideal strength and dynamic fracture.

Nanostructures We investigate the diffusion processes, growth, and atomic structure of metal and semiconductor surfaces and quantum dots using molecular dynamics simulations. We examine how the external environment can influence the atomic-scale processes that determine the structure of surfaces and quantum dots.

Quantum Computing A broad program is underway to use single-electron quantum dots in silicon for quantum information processing. A theoretical description of this system is necessarily multiscale, ranging from density functional theory at the atomic level to time-dependent model Hamiltonian calculations of many-dot systems. Optimal designs to minimize decoherence will be examined.

Quantum Dots This research is focused on optical, magnetic, and transport properties of quantum dots, nanocrystals, and other nanostructures. New theoretical approaches are used to describe how these properties are modified by nanoscale confinement and to understand new physical effects that appear at this length scale.

Radiation in Matter We develop quantum-open-systems approaches for non-equilibrium electromagnetic interactions in quantum-confined electronic systems, in the presence of environmental relaxation and decoherence phenomena. The electronic systems of interest include atomic systems and energetic electron beams in crystals.

Superconductors The Center has been contributing to understanding of novel superconductors since the discovery of high-T_c superconductivity in 1986. In recent years our main interest has been in the non-cuprate superconductors — such as MgB_2, the Ru-based superconductors, and the fullerides — and in the search for new superconducting materials. We are also interested in phenomena related to the interplay between superconductivity and magnetism.

Surfaces and Interfaces We investigate the physics of clean and adsorbed surfaces of semiconductors and metals. Reduced dimensionality plays an important role at surfaces, profoundly influencing electronic and magnetic properties. We also study the interfaces between materials, which are at the heart of technologically important phenomena such as grain-boundary formation, band-offset engineering, and spin injection.

POSTDOCTORAL PROGRAMS

Postdoctoral positions are available in the Center through the National Research Council and other programs. The annual stipends for Center postdocs in 2003 range from $40k to $55k.

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For more information about the Center and our research activities, plus our Publication Archive, visit **cst-www.nrl.navy.mil**

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Cover graphics (clockwise from upper left):
(1) $[Co(hmp)(CH_3OH)Cl]_4$ truncated rocksalt fragment, which forms a strongly anisotropic molecular ferromagnet; **(2)** Potential energy surface for adsorption of Mn on GaAs(001); **(3)** Electron charge density of a Mn impurity in Ge; **(4)** Radiative emission in a three-level atomic system; **(5)** Calculated susceptibility of Sr_2RuO_4; **(6)** Recently synthesized energetic octanitrocubane molecule with quartic vibrational mode; **(7)** A simulation of brittle fracture in silicon using coupling of length scales; **(8)** A highly correlated molecular vanadate many-spin system.

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MATERIALS SCIENCE AND TECHNOLOGY DIVISION

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